Specific heat of \mathbf{MgB}_2 in a one- and a two-band model from first-principles calculations

A A Golubov†, J Kortus‡, O V Dolgov‡, O Jepsen‡, Y Kong‡, O K Andersen‡, B J Gibson‡, K Ahn‡ and R K Kremer‡

†University of Twente, Department of Applied Physics, 7500 AE Enschede, The Netherlands ‡Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, D-70569 Stuttgart, Germany

E-mail: j.kortus@fkf.mpg.de

Abstract. The heat capacity anomaly at the transition to superconductivity of the layered superconductor MgB_2 is compared to first-principles calculations with the Coulomb repulsion, μ^* , as the only parameter which is fixed to give the measured T_c . We solve the Eliashberg equations for both an isotropic one-band and a two-band model with different superconducting gaps on the π -band and σ -band Fermi surfaces. The agreement with experiments is considerably better for the two-band model than for the one-band model.

Submitted to: J. Phys.: Condens. Matter

PACS numbers: 74.25B, 74.80Dm, 74.72.-h

1. Introduction

The nature of the superconducting state in MgB_2 has been characterized by a broad range of experimental and theoretical methods and many basic properties have been unambiguously established since the discovery of the $40 \, \text{K}$ superconductor MgB_2 by Nagamatsu and collaborators [1].

While electron-phonon coupling as the underlying pairing mechanism has been pinpointed by a large B isotope effect on T_c proving B related vibrations to be essential [2, 3] the nature of the order-parameter (viz. the superconducting gap) has remained a matter of debate. The order-parameter has been intensively investigated by tunnelling and point contact spectroscopy [4–16] as well as by high-resolution photoelectron spectroscopy [17, 18]. While these techniques show an energy gap in the quasiparticle spectrum most likely of s-wave symmetry the magnitude of the gap, $\Delta(0)$, itself remained an open question: tunnelling experiments initially revealed a distribution of energy gaps with lower boundary $2\Delta_1(0)/k_{\rm B}T_c \approx 1.1$ and upper boundary $2\Delta_2(0)/k_{\rm B}T_c \approx 4.5$. These values are either considerably lower or distinctly larger than the weak coupling BCS value of $2\Delta(0)/k_{\rm B}T_c = 3.53$ and these controversial findings have been discussed in terms of gap anisotropy or more recently attributed to the presence of two gaps or multiple gaps [12, 18]. The analysis of the electronic Raman continuum of MgB₂ by Chen et al. [13] also pointed to the presence of two gaps with gap values within the limits indicated by the tunnelling experiments [19].

While these experiments employ surface sensitive techniques to determine the gap properties, evidence for multigap behaviour emerges also from methods like heat capacity or μSR measurements probing true bulk properties [20]. In the early heat capacity experiments the typical jump-like anomaly is seen at T_c the magnitude $\Delta C_p/T_c$ of which amounts at best to only about 70-80% of the value $1.43 \gamma^{N}(T_c)$ predicted by weak-coupling BCS theory [2, 21–25]. $\gamma^{\rm N}(T_c)$ is the Sommerfeld constant in the normal state which was obtained from heat capacity measurements in high magnetic fields and which was determined to be 2.7-3 mJ mol⁻¹ K⁻². The shape of the heat capacity anomaly compares reasonably well with BCS-type behaviour assuming $2\Delta(0)/k_BT_c = 3.53$ with appropriately adjusted magnitude. An improved fit of the detailed temperature dependence of the heat capacity anomaly was obtained when calculating the heat capacity within the α -model [26] assuming a BCS temperature dependence of the gap but with an increased ratio $2\Delta(0)/k_BT_c = 4.2(2)$ [21]. This result matches very well with the upper limit of the gap value consistently found in the tunnelling experiments and was suggested as an evidence that MgB₂ is in the moderately strong coupling limit. More recently, the excess heat capacity observed close to $T_c/4$ by Bouquet et al. [22] and Wang et al. [24] has been attributed to a second smaller gap. Fits with a phenomenological two-gap model assuming that the heat capacity of MgB₂ can be composed as a sum of the two individual heat capacities gave very good description with gap values of $2\Delta_1(0)/k_BT_c = 1.2(1)$ and $2\Delta_2(0)/k_BT_c \approx 4$ [27]. Recent muon-spin-relaxation measurements of the magnetic penetration depth are consistent with a two-gap model [28].

Theoretically multigap superconductivity in MgB₂ was first proposed by Shulga et al.

to explain the behaviour of the upper critical magnetic field [29]. Based on the electronic structure the existence of multiple gaps has been suggested by Liu et~al. in order to explain the magnitude of T_c [30]. The electronic structure of MgB₂ contains four Fermi surface sheets [31]. Two of them with 2D character emerging from bonding σ bands form small cylindrical Fermi surfaces around Γ - A. The other two originating from bonding and antibonding π bands have 3D character and form a tubular network. Liu et~al. from first-principles calculations of the electron-phonon coupling conclude that the superconducting gap is different for the individual sheets and they obtain two different order parameters, a larger one on the 2D Fermi surface sheets and a second gap on the 3D Fermi surfaces, the latter was estimated to be approximately a factor of three reduced compared to the former [30].

In the present paper we calculate the specific heat capacity from the spectral Eliashberg function $\alpha^2(\omega)F(\omega)$ first in the one-band model using the isotropic $\alpha^2(\omega)F(\omega)$ as given by Kong et~al. [32]. Then we calculate the heat capacity in a two-band model by reducing the 16 Eliashberg functions $\alpha_{ij}^2(\omega)F_{ij}(\omega)$ appropriate for the four Fermi surface sheets into four Eliashberg functions corresponding to an effective-two-band model with a σ -band and π -band only. From the solution of the Eliashberg equations we obtain a superconducting gap ratio $\Delta_{\sigma}/\Delta_{\pi} \simeq 2.63$ in good agreement with the experimental data. The two-band model explains the reduced magnitude of the heat capacity anomaly at T_c very well and also reproduces the experimental observed excess heat capacity at low temperatures.

2. Theory

2.1. One-Band Model

First we discuss the specific heat in the isotropic single band model with a strong (intermediate) electron-phonon interaction (EPI). In the normal state and in the adiabatic approximation the electronic contribution to the specific heat is determined from the Eliashberg function $\alpha^2(\omega)F(\omega)$ by the expression [33]

$$C_N^{el}(T) = (2/3)\pi^2 N(0)k_B^2 T$$

$$\times \left[1 + (6/\pi k_B T) \int_0^\infty f(\omega/2\pi k_B T) \alpha^2(\omega) F(\omega) d\omega \right],$$
(1)

where N(0) is a bare density of states per spin at the Fermi energy. The kernel f(x) is expressed in terms of the derivatives of the digamma function $\psi(x)$

$$f(x) = -x - 2x^2 \operatorname{Im} \psi'(ix) - x^3 \operatorname{Re} \psi''(ix).$$
 (2)

At low temperatures the specific heat has the well known asymptotic form: $C_N^{el}(T \to 0) = (1+\lambda)\gamma_0 T$, where $\lambda = 2\int_0^\infty d\omega \, \omega^{-1}\alpha^2(\omega) F(\omega)$ is the electron-phonon coupling constant, and $\gamma_0 = 2\pi^2 k_B^2 N(0)/3$ is the specific heat coefficient for noninteracting electrons. At higher temperatures the specific heat differs from this trivial expression (see, the discussion in reference [34]).

In the superconducting state an expression for the specific heat obtained by Bardeen and Stephen [35] which is based on an *approximate* sum rule has often been used. We shall

however use an *exact* expression for the thermodynamical potential in the electron-phonon system which is based on the integration of the electronic Green's function over the coupling constant

$$\Omega = \Omega_{\rm el}^{(0)} + \Omega_{\rm ph}^{(0)} + T \sum_{\omega_{\rm n}} \int_{0}^{1} \frac{\mathrm{d}x}{x} \operatorname{tr} \left[\hat{\Sigma}(x) \hat{G}(x) \right]$$
(3)

where x is dimensionless, $\hat{G}(x)$ and $\hat{\Sigma}(x)$ are the exact electron Green's function and the self-energy, respectively, for a coupling constant of $x \cdot \lambda$. The functions $\Omega_{\rm el}^{(0)}$ and $\Omega_{\rm ph}^{(0)}$ are the thermodynamic potentials for noninteracting electrons and noninteracting phonons, respectively. Some further arithmetics leads to the expression for the difference in free energies, $F_{\rm N}$ and $F_{\rm S}$, of the superconducting and normal state [36]

$$-\frac{F_N - F_S}{\pi N(0)T} = \sum_{n = -\omega_c}^{\omega_c} \left\{ \begin{array}{l} |\omega_n| (Z^N(\omega_n) - 1) - \frac{2\omega_n^2 [(Z^S(\omega_n))^2 - 1] + \varphi_n^2}{|\omega_n| + \sqrt{\omega_n^2 (Z^S(\omega_n))^2 + \varphi_n^2}} \\ + \frac{\omega_n^2 Z^S(\omega_n) (Z^S(\omega_n) - 1) + \varphi_n^2}{\sqrt{\omega_n^2 (Z^S(\omega_n))^2 + \varphi_n^2}} \end{array} \right\}, \quad (4)$$

where $Z(\omega_n)$ is a normalization factor, $\varphi_n = \Delta_n/Z(\omega_n)$ is an order parameter, and Δ_n is the gap function.

The specific heat at temperature, T, is calculated according to:

$$\Delta C_{\rm el}(T) = T\partial^2(F_N - F_S)/\partial T^2. \tag{5}$$

The specific heat jump $\Delta C_{\rm el}(T_c)$ at $T=T_c$ is determined by the coefficient $\beta=T_c\Delta C_{\rm el}(T_c)/2$ in $F_N-F_S=\beta t^2$, where $t=(T_c-T)/T_c$.

2.2. Two-Band Model

We have calculated the 16 Eliashberg functions $\alpha_{ij}^2(\omega)F_{ij}(\omega)$ where i and j label the four Fermi surface sheets and thereafter combined them into four corresponding to an *effective* two-band model which contains only a σ - and π -band. Their respective densities of states at the Fermi energy have values of $N_{\sigma}(0)=0.300$ states/cell·eV and $N_{\pi}(0)=0.410$ states/cell·eV. Similar coupling constants $\lambda_{\sigma\sigma}, \lambda_{\pi\pi}, \lambda_{\sigma\pi}$, and $\lambda_{\pi\sigma}$ which are required for a two-band model were calculated earlier in reference [30]. The procedure of reducing the 16 Eliashberg functions of the real 4 band system due to the 4 different Fermi surface sheets to an effective two-band model with only four coupling constants λ_{ij} is an approximation which is based on the similarity of the two cylindrical and the two three-dimensional sheets of the Fermi surface requiring the same physical properties in both σ -bands or both π -bands. More details can be found elsewhere [37].

The four Eliashberg functions $\alpha_{ij}^2(\omega)F_{ij}(\omega)$ for the effective two-band model are shown in figure 1. The most significant contribution comes from the coupling of the bond stretching phonon modes to the σ -band. The coupling constants corresponding to the superconducting Eliashberg functions have been calculated to be: $\lambda_{\sigma\sigma}=1.017, \lambda_{\pi\pi}=0.448, \lambda_{\sigma\pi}=0.213,$ and $\lambda_{\pi\sigma}=0.155$. The small difference to the values given in reference [30] may be attributed to the different first-principles methods used in the calculation of the Eliashberg functions.

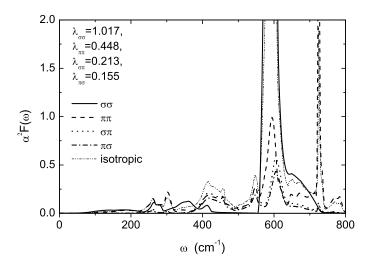


Figure 1. The four superconducting Eliashberg functions $\alpha^2 F(\omega)$ obtained from first-principles calculations for the effective two-band model and the isotropic Eliashberg function for the one-band model. The coupling constant of the isotropic one-band model has a value of λ_{iso} =0.87.

Besides the spectral functions we need to know the the Coulomb matrix element μ_{ij} . With the help of the wavefunctions from our first-principles calculations we can approximately calculate the ratios for the μ -matrix [37]. The $\sigma\sigma$ -, $\pi\pi$ - and $\sigma\pi$ -values were in the ratio 2.23/2.48/1. This allows one to express $\mu_{ij}^*(\omega_c)$ by these ratios and one single free parameter which is fixed to get the experimental T_c of 39.4 K from the solution of the Eliashberg equations. The $\mu^*(\omega_c)$ matrix elements determined by this procedure are $\mu^*_{\sigma\sigma}(\omega_c)$ =0.210, $\mu^*_{\sigma\pi}(\omega_c)$ =0.095, $\mu^*_{\pi\sigma}(\omega_c)$ =0.069, and $\mu^*_{\pi\pi}(\omega_c)$ =0.172.

Using our calculated Eliashberg functions on the imaginary (Matsubara) axis together with the above matrix $\mu_{ij}^*(\omega_c)$ we obtain the gap values $\Delta_{\sigma} = \lim_{T \to 0} \Delta_{\sigma}(i\pi T) \simeq 7.1$ meV, and $\Delta_{\pi} \simeq 2.7$ meV, which corresponds to $2\Delta_{\sigma}/k_BT_c$ =4.18 and $2\Delta_{\pi}/k_BT_c$ =1.59. The temperature dependence of the superconducting gaps is shown in figure 2. The filled circles (squares) display the gap for the 2D σ - (3D π -) band. Due to interband coupling between the bands both gaps close at the same critical temperature. For a comparison also the BCS curve (line) is shown for a single gap (one-band model) which closes at T_c =39.4 K. The corresponding single BCS gap would be 6 meV.

The extension of equation 1 to the two-band model gives

$$C_{\rm el}^{\rm N}(T) = \frac{2\pi^2}{3} N_{tot}(0) k_B^2 T + 4\pi k_B [N_{\sigma}(0)(I_{\sigma\sigma} + I_{\sigma\pi}) + N_{\pi}(0)(I_{\pi\pi} + I_{\pi\sigma})]$$
(6)

where $I_{ij} = \int_0^\infty f(\omega/2\pi k_B T) \alpha_{ij}^2(\omega) F_{ij}(\omega) d\omega$ $(i, j = \pi, \sigma)$, and the function f(x) is given by equation 2.

The generalization of the superconducting free energy (4) to the two band model is straightforward and the heat capacity was obtained according to equation 5.

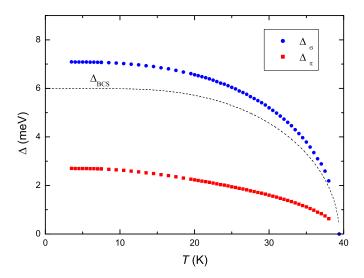


Figure 2. The temperature dependence of the the superconducting gaps from the solution of the two-band Eliashberg equations. The values of the gaps at T=0 K were obtained as Δ_{σ} (T = 0) = 7.1 meV and Δ_{π} (T = 0) = 2.7 meV. The BCS value for the gap that corresponds to T_c =39.4 K is 6.0 meV at 0 K.

3. Comparison with Experiment

For the comparison with experiment we have selected data obtained by our group [21] and by Bouquet et~al. [22]. The anomaly clearly visible at T_c in the zero-field data is suppressed by a magnetic field of 9 Tesla in both experiments. In figure 3 we display the difference $\Delta C_p = C_p(0 \mathrm{Tesla}) - C_p(9 \mathrm{Tesla})$. The anomalies at T_c detected by both groups clearly have a different magnitude, the one described in reference [22] amounts to 133 mJ/mol K at T_c and represents the largest specific heat capacity anomaly reported for MgB2 so far [38]. The $\Delta C_p(T_c)$ reported by our group is somewhat smaller, however, the shape of the anomalies close to T_c is very similar for both samples. In fact, fitting the anomalies with the α -model revealed an identical ratio $2\Delta/k_BT_c$ =4.2 with Δ =7 meV for both samples [21, 22, 27].

First we will try to discuss the experimental results in terms of a conventional one-band model. The specific heat in MgB₂ was calculated using the isotropic spectral Eliashberg function $\alpha^2(\omega)F(\omega)$ of Kong *et al.* [32]. This function yields an electron-phonon coupling constant $\lambda=0.87$ and together with a Coulomb pseudopotential of $\mu^*=0.1$ yields $T_c=40$ K. The calculated specific heat at T_c is $\gamma^N(T_c)=1.94\gamma_0=3.24$ mJ/mol K² with $\gamma_0=1.67$ mJ/mol K² from the band structure calculations of reference [31,32]. The specific heat jump at T_c equals $\Delta C \simeq 196$ mJ/mol K, which is a factor of 1.5-2 larger than the experimental values [38]. It corresponds to $\Delta C/(\gamma^N(T_c)T_c) \simeq 1.51$ compared to the BCS value of 1.43. The difference $\Delta C_{\rm el}(T) = C_{\rm el}^S(T) - C_{\rm el}^N(T)$ is shown in figure 3 (dashed-dot line) in comparison with the experimental data. Not only the size of the jump disagrees with the experiment, but also the behaviour at low temperatures is different. The latter is connected

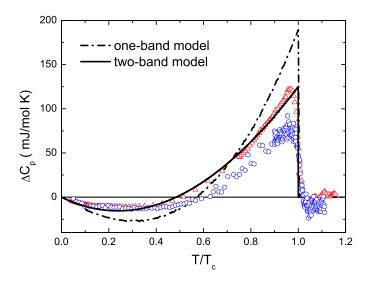


Figure 3. Experimental data of the heat capacity difference $\Delta C_p = C_p(0 \mathrm{Tesla}) - C_p(9 \mathrm{Tesla})$ from reference [21] (\circ) and from reference [22] (\triangle). The dashed line is the theoretical result of the one-band model and the thick solid line corresponds to the two-band model from the solution of the Eliashberg equations. The two-band model reproduces much better the specific heat jump as well as the low temperature behaviour.

with the fact that at low temperature equation (4) for a single band model leads to the standard exponential dependence $C^S \sim T^{-3/2} \exp(-\Delta/T)$, while the experimental data show a more complicated behaviour. Clearly there exists a discrepancy between experimental data and a theoretical one-band model.

The solid line in figure 3 represents the theoretical results for the two-band model as described above. The low temperature behaviour is in much better agreement with the experiment. The specific heat jump is now significantly reduced in comparison with a single band model and reproduces surprisingly well the experimental data of reference [22]. With the data given above we obtain from our theoretical calculation an electronic heat capacity in the normal state of $\gamma^{\rm N}(T_c) = C_{\rm el}^{\rm N}(T_c)/T_c \simeq 3.24~{\rm mJ/mol~K^2}$, the same value as for the one-band model. The absolute value of the specific heat jump in the two-band model is $\Delta C \simeq 125~{\rm mJ/mol~K}$, corresponding to $\Delta C/(\gamma^{\rm N}(T_c)T_c) \simeq 0.98$ which is now smaller than the BCS value.

We would like to emphasize here that no fitting is involved in the theoretical calculations. The only free parameter which is in the Coulomb matrix elements is already determined by the experimental T_c of 39.4 K.

One could expect that the difference between the theoretical results of the effective twoband model and our experimental data may be attributable to a different amount of impurities in the samples compared to the samples of reference [22]. In the one-band model the critical temperature T_c as well as the value and the temperature dependence of $\Delta C_p(T)$ are not affected by non-magnetic impurities (Anderson theorem). This is in complete contrast to the situation for the two-band model, where both quantities are strongly dependent on *interband* impurity scattering. Interband impurity scattering leads to averaging of the gaps and thus to the increase of $\Delta C_p/\gamma^{\rm N}(T_c)T_c$ ratio. On the other hand, due to decrease of T_c , the specific heat jump only depends weakly on the scattering strength. In order to investigate the dependence of T_c and of ΔC_p on the interband impurity scattering we included the effect of interband impurities in the Eliashberg equations. The results show that even for rather strong impurity scattering $1/2\tau=3\pi T_{c0}\simeq 371$ K, which leads to a drastic change of the critical temperature (decreasing to T_c =29.4 K) and strong averaging of the gaps, the specific heat jump remains practically unchanged $\Delta C_p\simeq 120$ mJ/mol K. This corresponds to a ratio $\Delta C_p/\gamma(T_c)T_c\simeq 1.48$, which is very close to the corresponding value of a single gap model. Therefore, interband impurity scattering can explain the change of T_c in different samples, but is not responsible for the observed different values of the specific heat capacity anomaly at T_c .

We have shown that a complete theoretical calculation from first-principles using an effective two-band model can explain the major features in the specific heat measurement of MgB_2 surprisingly well. The presented theoretical framework goes beyond a simple phenomenological two-gap model because interband effects are included explicitly and no fitting to experimental results has been performed. The reduced value of the heat capacity anomaly at T_c as well as the low temperature behaviour are in excellent agreement with experimental results. The same first-principles approach using exactly the same Eliashberg functions and Coulomb matrix elements has been used in order to explain optical measurements [37] and tunnelling experiments [40] of the interesting superconductor MgB_2 .

Acknowledgments

JK would like to thank the Schloeßmann Foundation for financial support.

References

- [1] Akimitsu J, Symposium on Transition Metal Oxides, January 2001, Sendai; Nagamatsu J, Nakagawa N, Muranaka T, Zenitani Y and Akimitsu J 2001 *Nature (London)* **410**, 63
- [2] Bud'ko S L, Lapertot G, Petrovic C, Cunningham C E, Anderson N and Canfield P C 2001 *Phys. Rev. Lett.* **86**, 1877
- [3] Hinks D G, Claus H and Jorgensen J D 2001 Nature (London) 411, 457
- [4] Karapetrov G, Iavarone M, Kwok W K, Crabtree G W and Hinks D G 2001 Phys. Rev. Lett. 86, 4374
- [5] Schmidt H, Zasadzinski J F, Gray K E and Hinks D G 2001 Phys. Rev. B 63, 220504 (R)
- [6] Rubio-Bollinger G, Suderow H and Vieira S 2001 Phys. Rev. Lett. 86, 5582
- [7] Sharoni A, Felner I and Millo O 2001 *Phys. Rev.* B **63**, 220508
- [8] Kohen A and Deutscher G 2001 Phys. Rev. B 64, 060506 (R)
- [9] Plecenik A, Beňačka Š, Kúš P and Grajcar M 2001 Preprint cond-mat/0104038
- [10] Szabó P, Samuely P, Kacmarcik J, Klein T, Marcus J, Fruchart D, Miraglia S, Marcenat C and Jansen A G M 2001 Phys. Rev. Lett. 87, 137005
- [11] Giubileo F, Roditchev D, Sacks W, Lamy R and Klein J 2001 Preprint cond-mat/0105146
- [12] Giubileo F, Roditchev D, Sacks W, Lamy R, Thanh D X, Klein J, Miraglia S, Fruchart D, Marcus J and Monod P 2001 *Phys. Rev. Lett.* **87**, 177008

- [13] Chen C-T, Seneor P, Yeh N-C, Vasquez R P, Jung C U, Park M-S, Kim H-J, Kang W N and Lee S-I 2001 *Preprint* cond-mat/0104285
- [14] Laube F, Goll G, Hagel J, v. Löhneysen H, Ernst D and Wolf T 2001 Europhys. Lett. 56, 296-301
- [15] Zhang Y, Kinion D, Chen J, Hinks D G, Crabtree G W and Clarke J 2001 Preprint cond-mat/0107478
- [16] Bugoslavsky Y, Miyoshi Y, Perkins G K, Berenov A V, Lockman Z, MacManus-Driscoll J L, Cohen L F and Caplin A D 2001 Preprint cond-mat/0110296
- [17] Takahashi T, Sato T, Souma S, Muranaka T and Akimitsu J 2001 Phys. Rev. Lett. 86, 4915
- [18] Tsuda S, Yokoya T, Kiss T, Takano Y, Togano K, Kitou H, Ihara H and Shin S 2001 *Phys. Rev. Lett.* **87**, 177006
- [19] Chen X K, Konstantinovič M J, Irwin J C, Lawrie D D and Franck J P 2001 Phys. Rev. Lett. 87, 157002
- [20] Heat capacity experiments are a classical tool to identify multiple gaps in superconductors. For example, strong evidence for two energy gaps has been gained from heat capacity measurements on high purity crystals of the the elemental superconductors Nb, Ta and V, cf. Meservey R and Schwartz B B in: *Superconductivity*, ed. by R.D. Parks (Maccel Dekker, Inc., NY, 1969) and reference to original works therein.
- [21] Kremer R K, Gibson B J and Ahn K 2001 Preprint cond-mat/0102432
- [22] Bouquet F, Fisher R A, Phillips N E, Hinks D G and Jorgensen J D 2001 Phys. Rev. Lett. 87, 047001
- [23] Wälti C, Felder E, Degen C, Wigger G, Monnier R, Delley B and Ott H R 2001 Phys. Rev. B 64, 172515
- [24] Wang Y, Plackowski T and Junod A 2001 Physica C, 355, 179
- [25] Yang H D, Lin J-Y, Li H H, Hsu F H, Liu C J and Jin C 2001 Phys. Rev. Lett. 87, 167003
- [26] Padamsee H, Neighbor J E and Shifman C A 1973 J. Low Temp. Phys. 12, 387
- [27] Bouquet F, Wang Y, Fisher R A, Hinks D G, Jorgensen J D, Junod A and Phillips N E 2001 Europhys. Lett. **56**, 856
- [28] Niedermayer C, Bernhard C, Holden T, Kremer R K and Ahn K 2001 Preprint cond-mat/018431
- [29] Shulga S V, Drechsler S-L, Eschrig H, Rosner H and Pickett W E 2001 Preprint cond-mat/0103154
- [30] Liu A Y, Mazin I I and Kortus J 2001 Phys. Rev. Lett. 87, 087008
- [31] Kortus J, Mazin I I, Belashchenko K D, Antropov V P and Boyer L L 2001 Phys. Rev. Lett. 86, 4656
- [32] Kong Y, Dolgov O V, Jepsen O and Andersen O K 2001 Phys. Rev. B 64, 020501 (R)
- [33] Grimvall G 1981 Electron-Phonon Interaction in Metals, (North-Holland, Amsterdam)
- [34] Shulga S V, Dolgov O V and Mazin I I 1992 Physica C 192, 41
- [35] Bardeen J and Stephen M 1964 Phys. Rev. 136, A1485
- [36] Golubev D A and Dolgov O V 1993 unpublished
- [37] Kuz'menko A B *et al* 2001 *Preprint* cond-mat/0107092, Solid State Commun. in press 2002; Dolgov O V *et al* 2002 to be published
- [38] It is interesting that experiments on different samples show similar values for the specific heat jump $\Delta C \simeq 113 \text{mJ/mol K}$ [2], $\Delta C \simeq 81 \text{mJ/mol K}$ [24], $\Delta C \simeq 133 \text{mJ/mol K}$ [22], $\Delta C \simeq 125 \text{mJ/mol K}$ [39] K = 125 mJ/mol K [23], $\Delta C \simeq 115 \text{mJ/mol K}$ [25], $\Delta C \simeq 92 \text{mJ/mol K}$ [39]
- [39] Frederick N A et al 2001 Physica C 363, 1
- [40] Brinkman A, Golubov A A, Rogalla H, Dolgov O V and Kortus J 2001 Preprint cond-mat/0111115